LLNL-CONF-608818

A Demonstration of the Disposal Systems Evaluation Framework (DSEF)

H. R. Greenberg, J. A. Blink, M. Sharma, M. Sutton

December 20, 2012

International High-Level Radioactive Waste Management Conference
Albuquerque, NM, United States
April 28, 2013 through May 2, 2013

Disclaimer

A Demonstration of the Disposal Systems Evaluation Framework (DSEF)*

Harris R. Greenberg, James A. Blink, Mark Sutton, and Montu Sharma
Lawrence Livermore National Laboratory
Corresponding author's email address: greenberg6@llnl.gov

LLNL-CONF-608818

ABSTRACT

The Disposal Systems Evaluation Framework (DSEF) is being developed at Lawrence Livermore National Laboratory (LLNL) to formalize and facilitate the development and documentation of repository conceptual design options for a range of waste forms, geologic environments, repository design concepts, and repository operating modes.

It is a knowledge management system that allows the user to intelligently access and draw data from a case library of hundreds of completed thermal analyses (currently 300 cases in the library), and draw input from databases of material properties and repository development cost data (currently the data in these databases is drawn from more than 100 references).

The core functionality of DSEF is provided by a Microsoft Office Excel 2010 workbook with macros and form controls that create a structured environment. The workbook walks the user through the steps of creating the input data required to perform disposal system evaluations by interfacing with external programs. The user can choose to work with built-in data from the case library of previous analysis cases, from the material property databases, or can define their own input descriptions and data.

DSEF is set up to retrieve the results of external program runs, summarize them graphically, and provide a template for adding the new results to the Case Library.

One of the key objectives of DSEF is to allow the user to compare the results of thermal analyses to thermal constraints of the waste forms, as well as the components of the natural and engineered barriers. These comparisons can then be used to consider design, layout, and operating mode modifications to find combinations that can meet the thermal constraints for a given set of waste forms, geologic media, surface storage times, and system operations.

The presentation will consist of a demonstration of the DSEF Excel workbook component, including thermal analysis component results from the Mathcad thermal analytical model.

INTRODUCTION

This paper provides the background and a description of the structure and information flow of DSEF. However, the conference presentation will be a live demonstration of the capabilities and use of the current version of the DSEF software.

The primary purpose of DSEF is to help the user tackle a multi-dimensional set of alternatives and options to arrive at workable potential high-level radioactive waste repository concepts. Figure 1 gives a small sense of the multi-dimensional nature of the problem.

For each combination of surface storage time, fuel cycle, and geologic media there are multiple Engineered Barrier System (EBS) design concept options for (1) Waste package spacing; (2) Waste package capacity; (3) Drift / borehole spacing; (4) EBS components, radii, and material properties.

There are many options to deal with and much input data for all of the analysis cases. DSEF helps the user take advantage of previous analyses to define potential new configurations and analysis cases that can meet the design and operating constraints.

Figure 2 shows a high level view of the inputs, the process, and the outputs of DSEF.

*This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

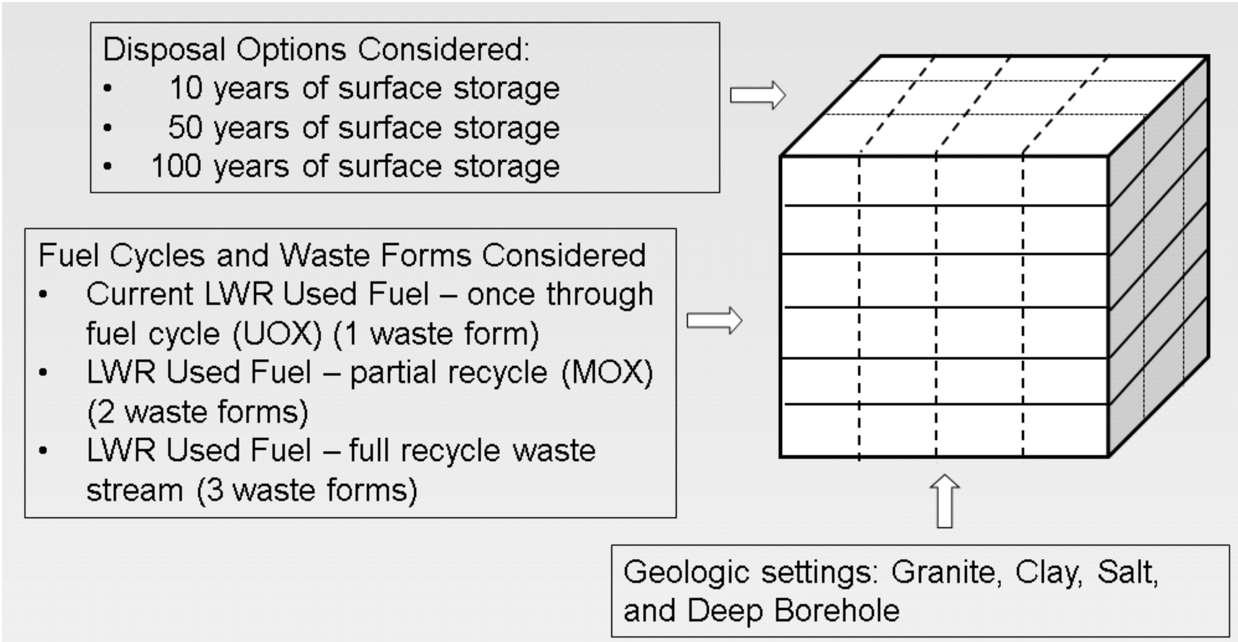

Figure 1. The Multi-Dimensional Problem

INPUTS

- **GEOLOGIC MEDIA DATA** HOST ROCK TYPE AND MATERIAL PROPERTIES
- **WASTE FORM PHYSICAL DATA** WASTE PACKAGE DIMENSIONS AND MATERIALS
- **WASTE FORM RADIOLOGICAL DATA** DECAY HEAT DATA BASED ON RADIONUCLIDE INVENTORY
- **ENGINEERED BARRIERS SYSTEM DATA** EBS LAYERS, MATERIAL TYPES, DIMENSIONS AND MATERIAL PROPERTIES
- **REPOSITORY LAYOUT CONCEPTS** PHYSICAL SPACING AND ARRANGEMENT DATA
- **STORAGE AND OPERATIONAL DATA** SURFACE STORAGE PRIOR TO EMPLACMENT, AND ASSUMPTIONS FOR OPERATIONS AND CLOSURE
- **CASE LIBRARY DATABASE** PREVIOUS ANALYSIS CASE INPUT DATA AND RESULTS

PROCESS

- **DEFINE** THE ANALYSIS CASE PARAMETERS, ASSUMPTIONS, AND DESIGN CONSTRAINTS
- **ASSEMBLE** REQUIRED INPUTS FOR EACH CASE
- **DOCUMENT** PARAMETER SELECTIONS FOR EACH CASE
- **DEVELOP** RANGE OF UNCERTAINTIES FOR PARAMETER UNCERTAINTY ANALYSIS
- **VALIDATE** ANALYSIS RESULTS BY COMPARING ANALYTICAL AND FINITE ELEMENT MODEL CALCULATIONS
- **COMPARE** THERMAL RESULTS AGAINST DESIGN CONSTRAINTS
- **ITERATE** REVISE INPUT ASSUMPTIONS UNTIL CONSTRAINTS CAN BE MET

OUTPUT

- **ACCEPTABLE REPOSITORY DESIGN AND OPERATING CONCEPTS**
- **TEMPERATURE TRANSIENT RESULTS**
- **ROUGH ORDER OF MAGNITUDE COSTS***
- **PERFORMANCE ASSESSMENT RESULTS FOR THE REPOSITORY CONCEPT** **
- **OUTPUT DATA TO INTERFACE WITH OTHER EXTERNAL PROGRAMS**
- **OUTPUT DATA AND RESULTS TO MASTER CASE LIBRARY**

Notes:
** DSEF Version 2.0 currently includes only subsurface development costs.*
***Not currently implemented in DSEF VERSION 2.0.*

Figure 2. DSEF Input-Process-Output Diagram

DSEF INFORMATION FLOW EXAMPLE

Figure 3 is an information flow diagram that shows how DSEF can be used to identify feasible repository disposal concepts.

Worksheets on the left side of the diagram provide a structured input environment where the user can enter data, access a built in library of natural and engineered material properties, or use sets of data that were previously analyzed as a starting point to define a new analysis case.

The Case Library and Case Catalog

The Case Library includes a Case Catalog that clearly identifies and organizes the various previous repository thermal analysis cases, grouping them into (1) “Enclosed mode” cases where the emplacement drift or borehole is backfilled immediately after emplacing the waste; (2) “Open mode” cases where the repository remain open and ventilated before eventually backfilling and closing the repository; and (3) Parameter sensitivity studies. The user selects a particular case number, and then clicks on a macro button that resets the screen and jumps the user into the Case Library for examination of the detailed data associated with that case.

The Thermal-Interpolate worksheet has two tools that allow the user to compare and contrast thermal analysis cases in the Case Library to help approximate the effects of parameter changes. One tool can focus on specific parameters of a set of cases picked by the user for comparison purposes, and the other tool will provide interpolated analysis results based on a selection of independent and dependent variables.

Material Data Plotting and Material Properties Data

The Material Data Plotting worksheet only contains a short list of instructions and a “Click here to plot data distribution” macro button. After clicking on that macro button a “Select a Range” user input box appears. At this point, the user is free to navigate between material data worksheets by clicking on tabs at the bottom of the screen and then scrolling with the mouse to any set of data on those worksheets. The only restriction is that the range of data must be restricted to the yellow-highlighted columns, representing the high and low values of a single data parameter.

The range of data selected can be a continuous block of data values or a separate collection of different data sets (you can use the CTRL key with the mouse to select non-contiguous sets of data).

Any blank rows in the middle of a range of data will be ignored. After clicking “OK” on the range selection box, the user is returned to the Material Data Plotting worksheet to choose a location to place the statistical data and the plot, as shown in Figure 4. However, the user is not restricted to placing the output data and plot on this worksheet. They can be placed on any other worksheet by navigating to the new location before clicking OK to insert the plot.

The Interface to External Analysis Programs

The worksheets in the central area of Figure 3 are the ones that perform the calculations, or pass collected input data to external programs, and retrieve the output results from the external programs. DSEF is intended to interface with a wide variety of thermal analysis codes. The Mathcad thermal analytical model is fully implemented in DSEF, and other finite element model (FEM) thermal analyzer interface worksheets are under development. TrueGrid and DIABLO are shown as example FEM mesh generation and FEM thermal analysis codes, respectively. The Mathcad thermal analytical model was used to develop the existing set of data in the Case Library.

Comparison of Results to Design Constraints

The right-hand side of Figure 3 shows the comparison of results against design constraints, and the iteration process used if constraints are not met. Examples of design constraints are temperature limits of 100°C for a clay or granite repository concept (with bentonite buffers), or 200°C in salt. The 100°C temperature constraint was chosen to limit alteration of clay in buffers, for example by illitization or cementation. Alteration generally involves dissolution, aqueous transport, and precipitation. For salt, a more ductile material, a higher target value of 200°C is used for the maximum temperature, to limit uncertainty in performance assessment.

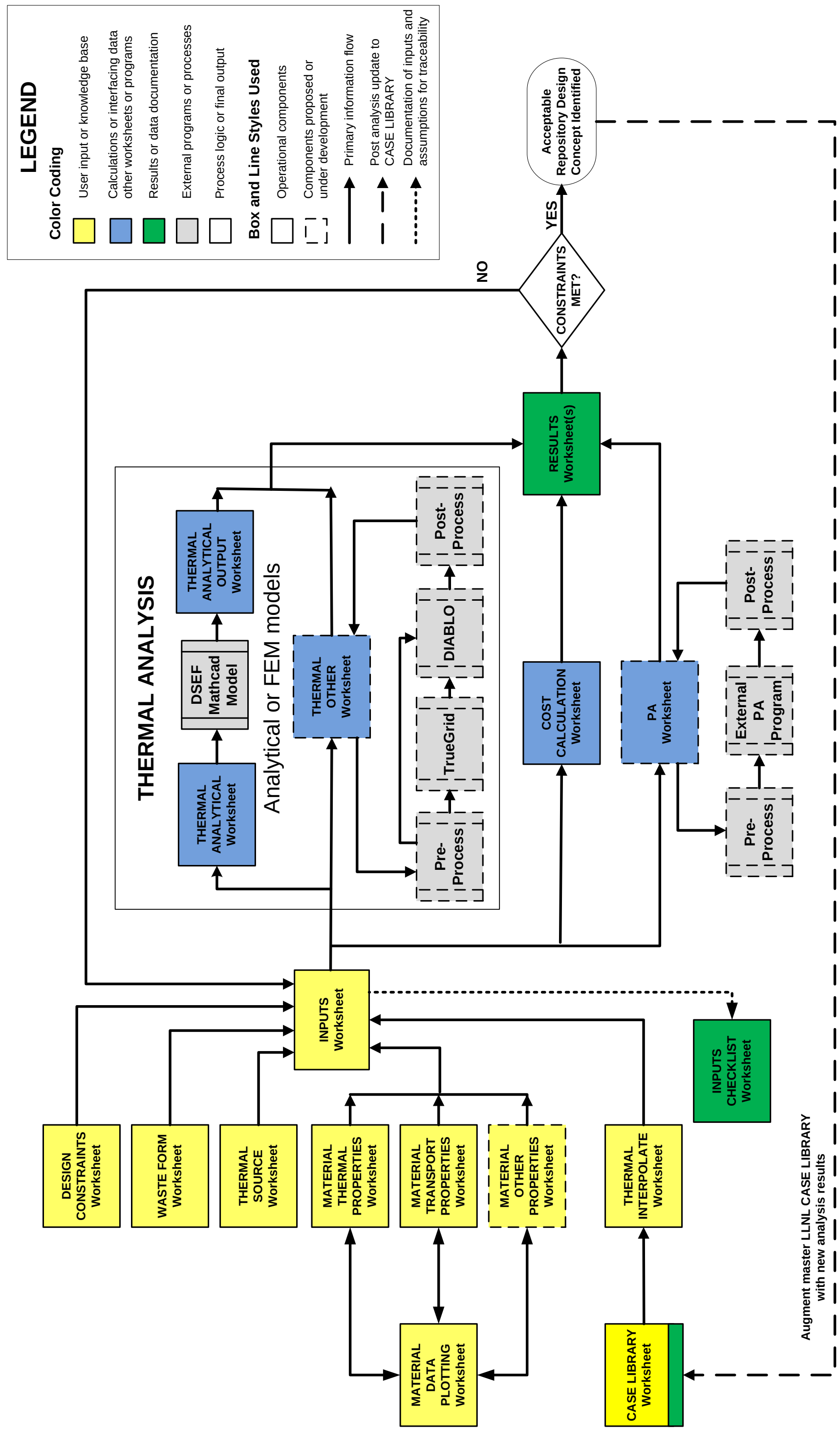

Figure 3. Information Flow Diagram for DSEF

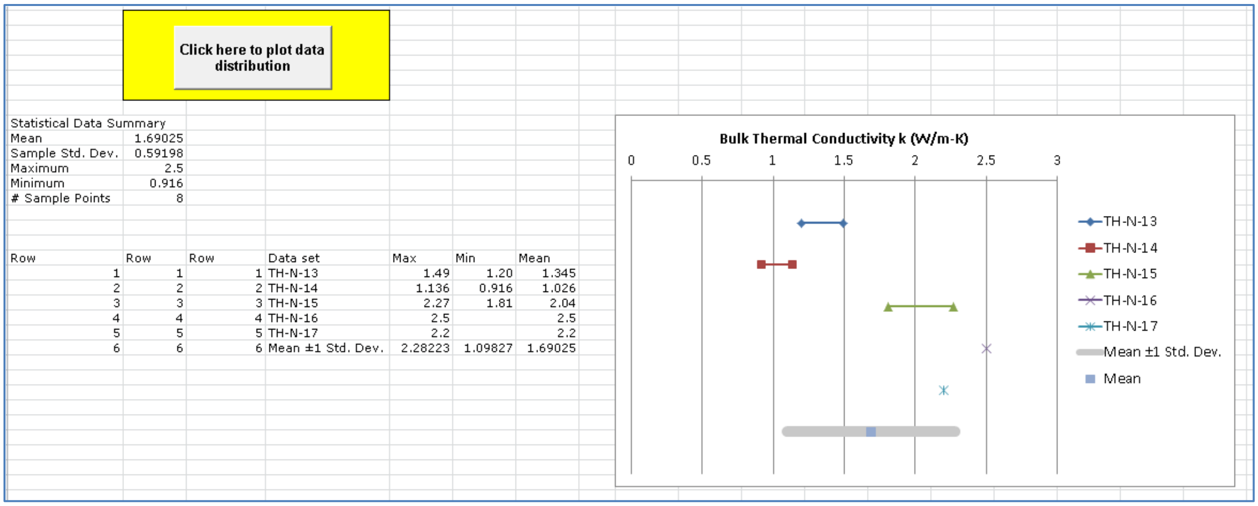

Figure 4. Example Output of the Materials Data Plotting Macro

CONCLUSIONS

DSEF was initially developed to support analysis efforts in 2011 [1] and [2], and was updated in 2012 [3]. More than 300 analysis cases of potential repository design and operating concepts are documented in the DSEF case library sheet and in [4], [5], and [6].

DSEF has been proven to be an effective tool for knowledge management of a large amount of scientific and engineering analysis data. It has helped to effectively leverage previous analyses to define new workable repository concepts for a wide range of geologic media, waste forms, and repository design concepts.

REFERENCES

1. M. Sutton, J. A. Blink, M. Fratoni, H. R. Greenberg, and A. D. Ross, *Investigations on Repository Near-Field Thermal Modeling*, LLNL-TR-491099 Rev. 1, Lawrence Livermore National Laboratory, December 2011

2. E. Hardin, J. Blink, H. Greenberg, M. Sutton, M. Fratoni, J. Carter, M. Dupont, and R. Howard, *Generic Repository Design Concepts and Thermal Analysis (FY11)*, SAND2011-6202, Sandia National Laboratories, August 2011

3. H. R. Greenberg, J. A. Blink, M. Sharma, and M. Sutton, *The Disposal Systems Evaluation Framework (DSEF) Version 2.0 User's Guide*, Lawrence Livermore National Laboratory, January 2013

4. H. R. Greenberg, M. Sharma, M. Sutton and A.V. Barnwell, *Repository Near-Field Thermal Modeling Update Including Analysis of Open Mode Design Concepts*, , LLNL-TR-572252, Lawrence Livermore National Laboratory, August 2012

5. H.R. Greenberg, M. Sharma, and M. Sutton, *Investigations on Repository Near-Field Thermal Modeling*, LLNL-TR-491099 Rev. 2, Lawrence Livermore National Laboratory, November 2012

6. E. Hardin, T. Hadgu, D. Clayton, R. Howard, H. Greenberg, J. Blink, M. Sharma, M. Sutton, J. Carter, M. Dupont and P. Rodwell, *Repository Reference Disposal Concepts and Thermal Load Management Analysis*, FCRD-UFD-2012-00219 Rev. 2, Sandia National Laboratories, November 2012